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Application of molecular modelling in heterogeneous catalysis research

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Traditionally, heterogeneous catalysis has largely been an experimental field. While this is still true today, it is increasingly recognized that computer modelling and simulation are important tools in the study and development of catalytic systems. Molecular modelling has the potential to provide new insights into reaction pathways, to predict properties of catalysts that have not yet been synthesized, and to bring information for a given system from many different experimental techniques into a coherent picture. A close interaction of modelling and experiment is vital. The most fruit-fully strategy for using modelling in catalysis research is likely to be a dual-feedback mode, where experiments (kinetic studies of reaction rates, thermodynamic information on adsorption, and spectroscopic data on molecular-level structure) are used to validate the modelling and modelling is used to explain experimental results, to suggest new experiments, and perhaps to substitute for experiments in the screening of different catalysts or reaction conditions. The objective of this work is to present the dual-feedback mode on three case studies from the branch of heterogeneous catalysis and to highlight some interesting outputs as a result of applying such approach. The first issued from the study of molecular structure effects on noble metal catalyst. It presents usefulness of such approach for probing the mechanism of surface processes in hydrogenation of CC unsaturated bonds. The second one demonstrates how could theoretical calculations help in characterizing of active site in cinchona modified platinum catalyst and also judged the mechanism theories in stereoselective hydrogenations. The last case study presents a possibility to predict properties of hydrotalcite catalyst used for aldolization of cyclic ketones before its synthesis and also to define its applicability.

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